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     FILE 'CAPLUS' ENTERED AT 13:54:11 ON 23 MAR 2004
                E CHMIELEWSKI JEAN/IN,AU
                E KAHR BERT/IN,AU
L1            1 S E2
                E CHMIELEWSKI JEAN/IN,AU
L2           63 S E4-7
                E LEWIS JERRY/IN,AU
L3           51 S E1-18
L4            0 S L1 AND L2 AND L3
L5          113 S L1 OR L2 OR L3
L6      1835784 S CRYSTAL?
L7       444761 S MATRIX
L8            7 S L5 AND (L6 OR L7)
L9            0 S 200:900424/AN
L10           1 S 2000:900424/AN
L11           1 S 1999:422851/AN
L12           1 S 1997:667182/AN
L13       44924 S LACTOSE
L14      436744 S CRYSTAL STRUCTURE
L15         186 S L13 AND L14
L16      230738 S SINGLE CRYSTAL
L17      444761 S MATRIX
L18      314285 S LATTICE
L19          20 S L15 AND (L16 OR L17 OR L18)
L20          18 S L19 NOT L8

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L8 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:411418 CAPLUS
DOCUMENT NUMBER: 135:43027
TITLE: Intrasectoral zoning of proteins and nucleotides in simple **crystalline** hosts
AUTHOR(S): Kurimoto, Miki; Bastin, Loyd D.; Fredrickson, Daniel; Gustafson, Pamela N.; Jang, Sei-Hum; Kaminsky, Werner; Lovell, Scott; Mitchell, Christine A.; **Chmielewski, Jean**; Kahr, Bart
CORPORATE SOURCE: Department of Chemistry, University of Washington, Seattle, WA, 98195-1700, USA
SOURCE: Materials Research Society Symposium Proceedings (2001), 620(Morphology and Dynamics of Crystal Surfaces in Complex Molecular Systems), M9.8.1-M9.8.10
CODEN: MRSPDH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Oriented gases of biopolymers in simple, single **crystal** hosts might be used to measure anisotropic mol. properties of analytes that could not otherwise be **crystd.** Here we show two types of **crystals** as examples of the single **crystal matrix** isolation of biopolymers: green fluorescent protein in α-lactose monohydrate as a model system for studying the kinetic stabilization of biopharmaceuticals, and adenosine phosphates in potassium dihydrogen phosphate, a first step in the **matrix** isolation of oligonucleotides. In each case, the hosts undergo compositional zoning - both intersectoral and intrasectoral - during growth from solution Intrasectoral zoning is evident by the selective luminescence of adjacent vicinal slopes of growth active hillocks. Nucleotides furthermore distinguish between symmetry related growth sectors enantioselectively.
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:900424 CAPLUS
DOCUMENT NUMBER: 134:46765
TITLE: Pharmaceuticals containing a **crystal** lattice component
INVENTOR(S): **Chmielewski, Jean A.**; Kahr, Bart E.; Lewis, Jerry
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000076480	A2	20001221	WO 2000-US16140	20000612
WO 2000076480	C2	20020711		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1189599	A2	20020327	EP 2000-939811	20000612
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: US 1999-138912P P 19990611
WO 2000-US16140 W 20000612

AB Pharmaceutical compns. comprising **crystals** of a pharmaceutically-acceptable **crystal** lattice component, and an active pharmaceutical ingredient different from and included within the **crystal** lattice component in a growth-sector specific orientation. The **crystals** are prepared using components and methods which yield **crystals** having suitable purity and efficacy for use in administering the active pharmaceutical ingredients to a patient. The **crystals** are typically combined with adjuvants such as excipients, diluents or carriers, and are preferably formulated into tablets,

capsules, suspensions, and other conventional forms containing predetd. amts. of the pharmaceuticals. Also provided are methods for preparing the **crystals**, and methods for storing and administering the active pharmaceutical ingredient either included within the **crystals** or upon reconstitution of the **crystals** to a solution The kinetic stabilization of proteins with lactose monohydrate was demonstrated.

L8 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:424967 CAPLUS
DOCUMENT NUMBER: 133:33721
TITLE: Compliance testing using EPA Method 0040 for VOCs (Sampling and Analysis of Volatile Organic Compounds Using Tedlar Bags)
AUTHOR(S): **Lewis, Jerry W.**; Sykes, Alston L.
CORPORATE SOURCE: Centroid Testing, Providence, NC, 27560, USA
SOURCE: Measurement of Toxic and Related Air Pollutants, Proceedings of a Specialty Conference, Cary, NC, United States, Sept. 1-3, 1998 (1998), Volume 1, 579-587. Air & Waste Management Association: Pittsburgh, Pa.
CODEN: 69AAKD
DOCUMENT TYPE: Conference
LANGUAGE: English
AB In June 1997, EPA SW-846 Method 0040 "Sampling of Principal Organic Hazardous Constituents from Combustion Sources Using Tedlar Bags" Revision 0, Jan. 1995, was approved for testing stationary sources. After EPA's approval, the method was used in the State of New Jersey for compliance demonstration of 1,3-butadiene and benzene at an industrial facility. The 0040 sampling equipment was purchased from a com. vendor and problems were encountered in meeting the required leak check criteria during the initial use. Modifications to the equipment were made that allowed subsequent leak checks to be met in a reasonable time. The method requires on-site spiking of the volatile organic compds. (VOCs) of interest to determine **matrix** effects and recovery efficiency. Deuterated compds. were used to spike the samples during this test, although not specifically required in the method. Because of the required level of experience necessary for performing these methods both in the field and laboratory, close communications must take place between the field testing firm, the laboratory, and the state agency. The sample train and GC/MS Tedlar bag anal. procedures provide a good alternative to the VOST Methods 0030 and 0031 and EPA Method 18. The most interesting aspects of Method 0040 are:. • Multiple analyses can be performed on each sample vs. only one with VOST. • Samples can be diluted into another Tedlar bag if high organic concns. are found. • A lower anal. cost per test compared to the VOST can be realized.
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:422851 CAPLUS
DOCUMENT NUMBER: 131:225027
TITLE: Kinetic Stabilization of Biopolymers in Single-**Crystal** Hosts: Green Fluorescent Protein in α-Lactose Monohydrate
AUTHOR(S): Kurimoto, Miki; Subramony, Paramjeet; Gurney, Richard W.; Lovell, Scott; **Chmielewski, Jean**; Kahr, Bart
CORPORATE SOURCE: Department of Chemistry, University of Washington, Seattle, WA, 98195-1700, USA
SOURCE: Journal of the American Chemical Society (1999), 121(29), 6952-6953
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors demonstrate that green fluorescent protein (GFP) can be oriented and stabilized in its native conformation in single **crystals** of α-lactose monohydrate, and subsequently release into solution in its native state by dissoln. of the **matrix**.
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

pub 7/28/99

L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:667182 CAPLUS
DOCUMENT NUMBER: 127:259706
TITLE: Single-**Crystal Matrix** Isolation of Biopolymers
AUTHOR(S): **Chmielewski, Jean; Lewis, Jerry J.**

; Lovell, Scott; Zutshi, Reena; Savickas, Phil; Mitchell, Christine A.; Subramony, J. Anand; Kahr, Bart
CORPORATE SOURCE: Department of Chemistry, Purdue University, West Lafayette, IN, 47907, USA
SOURCE: Journal of the American Chemical Society (1997), 119(43), 10565-10566
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This article demonstrates the incorporation and orientation of proteins and an oligonucleotide in host aromatic acid **crystals** using 3 imaging techniques:fluorescence microscopy/spectroscopy, single **crystal** desorption mass spectrometry, and autoradiog.

L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:805265 CAPLUS
DOCUMENT NUMBER: 124:30399
TITLE: Synthesis of the basic-helix-loop-helix region of the immunoglobulin enhancer binding protein E47 and evaluation of its structural and DNA binding properties
AUTHOR(S): Bishop, Patricia; Jones, Cory; Ghosh, Indraneel; **Chmielewski, Jean**
CORPORATE SOURCE: Department of Chemistry, Purdue University, West Lafayette, IN, USA
SOURCE: International Journal of Peptide & Protein Research (1995), 46(2), 149-54
CODEN: IJPPC3; ISSN: 0367-8377
PUBLISHER: Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The basic-helix-loop-helix (bHLH) region of the Ig enhancer binding protein E47 (IEB E47) was prepared in high yield by a solid-phase peptide synthesis methodol. Size-exclusion chromatog., sedimentation equilibrium and crosslinking data showed that the synthetic bHLH protein, 1, was dimeric, and higher-order aggregates of trimer and tetramer were also observed The CD spectrum of 1 showed a high helical content, which increased upon addition of DNA containing the κE2 sequence. Gel mobility shift expts. showed that protein 1 bound sequence specifically to the κE2 sequence with a binding constant of 10-10 M2, and had an affinity for other E box sequences as well. Comparisons between the co-**crystal** structure of IEB E47 with DNA and structural studies in solution showed lower helical contents in solution as would have been predicted from the **crystal** structure.

L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:120957 CAPLUS
DOCUMENT NUMBER: 90:120957
TITLE: An improved synthesis of diammonium acetyl phosphate
AUTHOR(S): **Lewis, Jerome M.**; Haynie, Sharon L.; Whitesides, George M.
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA
SOURCE: Journal of Organic Chemistry (1979), 44(5), 864-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB AcOP(O)(ONH4)2 was prepared on a >500 g scale by acylating 100% H3PO4 with Ac2O in AcOEt at 0° and adding the resulting mixture of mono- and polyacetylphosphoric acids to a solution of MeOH saturated with anhydrous NH3 at -10°. The product is obtained as an easily filtered, **cryst** . solid in .apprx.85% yield and purity.

L20 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:633276 CAPLUS
DOCUMENT NUMBER: 139:169334
TITLE: Anti-inflammatory androstane derivative compositions
INVENTOR(S): Biggadike, Keith; Coote, Steven John; Craig, Andrew S.; Jacewicz, Victor W.; Millan, Michael J.; Nice, Rosalyn K.; Noga, Brian M.; Seager, John F.; Theophilus, Andrew L.; Crowe, David M.
PATENT ASSIGNEE(S): UK
SOURCE: U.S. Pat. Appl. Publ., 66 pp., Cont.-in-part of U.S. Ser. No. 958,050.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 9
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003153542	A1	20030814	US 2002-67010	20020204
WO 2002012265	A1	20020214	WO 2001-GB3495	20010803
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003199485	A1	20031023	US 2001-958050	20011002
US 2003109511	A1	20030612	US 2002-200364	20020722
US 2003144257	A1	20030731	US 2002-241658	20020911
WO 2003066656	A1	20030814	WO 2003-GB478	20030204
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO 2003066033	A1	20030814	WO 2003-GB485	20030204
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:

GB 2000-19172	A	20000805
WO 2001-GB3495	A1	20010803
US 2001-958050	A2	20011002
GB 2001-8800	A	20010407
US 2002-66961	A	20020204
US 2002-67010	A2	20020204
US 2002-200364	A2	20020722

AB There is provided a crystalline composition comprising I in which the crystal **lattice** is stabilized by the presence of a guest mol. The crystalline composition is of space group P212121 having unit cell dimensions of about 12.1, 14.9, and 16.2 Å when determined at either 120K or 150K. Thus, I was prepared starting from 6α,9α-difluoro-11β,17α-dihydroxy-16α-methyl-3-oxo-androsta-1,4-diene-17β-carbothioic acid. Thus, a dry powder composition contained I solvate with acetone (MMD 3 μm) 0.20, and milled **lactose** 12 mg. A peelable blister strip containing 60 blisters each filled with a formulation described above is prepared

L20 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:493308 CAPLUS

DOCUMENT NUMBER: 137:295166
TITLE: Dehydration Mechanism and Crystallization Behavior of **Lactose**
AUTHOR(S): Garnier, S.; Petit, S.; Coquerel, G.
CORPORATE SOURCE: IRCOF, UPRES EA 2659, Unite de Croissance Cristalline et de Modelisation Moleculaire (UC2M2) Sciences et Methodes Separatives (SMS), Universite de Rouen, Mont Saint-Aignan, F-76821, Fr.
SOURCE: Journal of Thermal Analysis and Calorimetry (2002), 68(2), 489-502
CODEN: JTACF7; ISSN: 1418-2874
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dehydration mechanism of α- **lactose** monohydrate was investigated by several techniques and interpreted on the basis of structural data. Whatever the dehydration conditions (heating or use of hygroscopic organic solvents), the departure of water mols. occurs cooperatively in channels parallel to the c axis of the initial structure. Subsequently, the reorganization leads to the closest packing (hygroscopic metastable form, LαH) under heating or to the stable anhydrous form (LαS), probably via a nucleation and growth process in ethanol. The use of acetone as dehydrating solvent on **single crystals** of α- **lactose** monohydrate led to the unexpected formation of **single crystals** of the anomeric β- **lactose** at room temperature, from which the **crystal structure** of β- **lactose** could be accurately redetd. Recrystn. expts. of anhydrous **lactose** allowed to prepare N-methylpyrrolidinone and DMSO solvates of α- **lactose**.
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:897279 CAPLUS
DOCUMENT NUMBER: 136:184575
TITLE: Thermal and mechanical behaviors of poly(vinyl alcohol)-**lactose** blends
AUTHOR(S): Fan, Xiao-Dong; Hsieh, You-Lo; Krochta, John M.
CORPORATE SOURCE: Department of Chemical Engineering, Northwestern Polytechnic University, Xian, 710072, Peop. Rep. China
SOURCE: Journal of Applied Polymer Science (2002), 83(4), 929-935
CODEN: JAPNAB; ISSN: 0021-8995
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Thermal and mech. behaviors of poly(vinyl alc.) (PVA)-**lactose** blends were studied by differential scanning calorimetry, thermal gravimetric anal., and stress-strain anal. The increase in glass transition temperature of the PVA-**lactose** blends with **lactose** contents suggests the formation of hydrogen-bonded PVA-**lactose** complex in the PVA **matrix**. The hydrogen bonding interactions can improve thermal and mech. properties of the blends. Results of this study demonstrate that **lactose**, a byproduct of dairy industry, can be used directly and in substantial quantity (33%) as a modifier to enforce the phys. properties of PVA.
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:642070 CAPLUS
TITLE: Solution and solid state polymerization of 2,3-dicyano-5,7-dimethyl-6H-1,4-diazepine
AUTHOR(S): Kim, Ik-Bum; Foxman, Bruce M.; Njus, Jeffrey; Sandman, Daniel J.
CORPORATE SOURCE: Department of Chemistry, University of Massachusetts Lowell, Lowell, MA, 01854, USA
SOURCE: Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, United States, August 26-30, 2001 (2001), POLY-200. American Chemical Society: Washington, D. C.
CODEN: 69BUZP
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB We describe the polymerization of the dicyanoalkene, 2,3-dicyano-5,7-dimethyl-6H-1,4-diazepine(1), to high mol. weight conjugated polymers via two different new chemical methodologies that are nonpolluting, namely the use of unmodified carbohydrate reagents in solution and the use of solid state

reactions that use no solvent. The polymers that we prepare as described herein have not been previously prepared The polymerization of 1 has been investigated in solution and solid state, and conjugated polymers were prepared in both cases. Solution polymerization proceeds using unmodified sugar reagents, such as glucose, **lactose**, and sucrose, in alkaline methanol solution The solid state polymerization is thermally carried out at 150°C. A monoclinic unit cell was determined from the **crystal structure** of **single crystal** monomer (1) by X-ray crystallog. Structures are proposed for the polymer based on 1H and 13C NMR, IR, and UV-visible spectra and other techniques. Since the polymers from 1 are not sufficiently soluble to obtain 13C spectra in solution, these spectra were obtained using cross polarization and magic angle spinning (CPMAS) techniques. Their properties are under investigation.

L20 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:164274 CAPLUS
DOCUMENT NUMBER: 135:30827
TITLE: Copurification of the Lac Repressor with Polyhistidine-Tagged Proteins in Immobilized Metal Affinity Chromatography
AUTHOR(S): Owens, Roisin M.; Grant, Andrew; Davies, Nicholas; O'Connor, C. David
CORPORATE SOURCE: Division of Biochemistry and Molecular Biology, University of Southampton, Bassett Crescent East, SO16 7PX, UK
SOURCE: Protein Expression and Purification (2001), 21(2), 352-360
CODEN: PEXPEJ; ISSN: 1046-5928
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB One of the commonly used resins for immobilized metal affinity purification of polyhistidine-tagged recombinant proteins is TALON resin, a cobalt (II)-carboxymethylaspartate-based **matrix** linked to Sepharose CL-6B. Here, we show that TALON resin efficiently purifies the native form of Lac repressor, which represents the major contaminant when (His)6-tagged proteins are isolated from Escherichia coli host cells carrying the lacIq gene. Inspection of the **crystal structure** of the repressor suggests that three His residues (residues 163, 173, and 202) in each subunit of the tetramer are optimally spaced on an exposed face of the protein to allow interaction with Co(II). In addition to establishing a more efficient procedure for purification of the Lac repressor, these studies indicate that non-lacIq-based expression systems yield significantly purer prepns. of recombinant polyhistidine-tagged proteins. (c) 2001 Academic Press.
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:123334 CAPLUS
DOCUMENT NUMBER: 120:123334
TITLE: Synthesis and characterization of nickel(II) complexes containing ligands derived from disaccharides and 1,3-diaminopropane
AUTHOR(S): Tanase, Tomoaki; Nouchi, Reiko; Oka, Yukiko; Kato, Masako; Nakamura, Nobufumi; Yamamura, Takeshi; Yamamoto, Yasuhiro; Yano, Shigenobu
CORPORATE SOURCE: Fac. Sci., Toho Univ., Funabashi, 274, Japan
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1993), (17), 2645-52
CODEN: JCDTBI; ISSN: 0300-9246
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction of [Ni(tn)3]2+ ions (tn = 1,3-diaminopropane) with disaccharides having a glucose reducing terminal, i.e. maltose, **lactose**, cellobiose, and melibiose, in the presence of a catalytic amount of NH4Cl gave blue, paramagnetic bis(N-D-aldosylpropane-1,3-diamine)nickel(II) complexes. The complexes were characterized by elemental anal., magnetic susceptibilities, electronic absorption and CD spectroscopies, x-ray absorption and crystallog. analyses. Bis[N-(4-O-α-D-glucopyranosylglucosyl)propane-1,3-diamine]nickel(II) bromide dihydrate crystallizes in the hexagonal space group P6422, with a 22.125(8), c 21.464(9) Å, and Z = 6. The structure was solved by Patterson methods and refined by full-**matrix** least-squares techniques to R = 0.080 and R' = 0.094. The complex cation has C2 symmetry and the central Ni atom is octahedrally coordinated by 2 tridentate glycosylamine ligands formed from maltose and tn. Each ligand is bonded through the O atom of the hydroxyl group at C2 of maltose and

through the 2 N atoms of the diamine in a meridional mode. The coordination behavior of the glucose unit in the octahedral Ni(II) complexes was established. In the crystal packing, the complex cation exists in a novel dimeric form supported by intermol. H bonds, which might provide some fundamental information concerning sugar-sugar interactions in biol. systems.

L20 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:664850 CAPLUS
DOCUMENT NUMBER: 119:264850
TITLE: X-ray **crystal structure** of the human dimeric S-Lac lectin, L-14-II, in complex with **lactose** at 2.9-Å resolution
AUTHOR(S): Lobsanov, Yuri D.; Gitt, Michael A.; Leffler, Hakon; Barondes, Samuel H.; Rini, James M.
CORPORATE SOURCE: Dep. Mol. Med. Genet., Univ. Toronto, Toronto, ON, M5S 1A8, Can.
SOURCE: Journal of Biological Chemistry (1993), 268(36), 27034-8
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB S-Lac lectins are a family of soluble **lactose**-binding animal lectins, some of which have been implicated in modulating cell-cell and cell-**matrix** interactions through specific carbohydrate-mediated recognition. The authors report here the x-ray **crystal structure** of a representative member of this family, the human dimeric S-Lac lectin, L-14-II, in complex with **lactose**, at 2.9-Å resolution The two-fold sym. dimer is made up of two extended anti-parallel β-sheets, which associate in a β-sandwich motif. Remarkably, the L-14-II monomer shares not only the same topol., but a very similar β-sheet structure with that of the leguminous plant lectins, suggesting a conserved structure-function relationship. Carbohydrate binding by L-14-II was found to involve protein residues that are very highly conserved among all S-Lac lectins. These residues map to a single DNA exon, suggesting a carbohydrate binding cassette common to all S-Lac lectins.

L20 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:499125 CAPLUS
DOCUMENT NUMBER: 115:99125
TITLE: Elucidation of the compressive deformation behavior of α- **lactose** monohydrate and anhydrous α- **lactose single crystals** by mechanical strength and acoustic emission analyses
AUTHOR(S): Wong, D. Y. T.; Waring, M. J.; Wright, P.; Aulton, M. E.
CORPORATE SOURCE: Sch. Health Life Sci., Leicester Polytech., Leicester, LE1 9BH, UK
SOURCE: International Journal of Pharmaceutics (1991), 72(3), 233-41
CODEN: IJPHDE; ISSN: 0378-5173
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Compressive deformation studies on single α- **lactose** crystals by mech. strength and acoustic emission analyses revealed a distinct difference in the deformation behavior of α- **lactose** monohydrate and anhydrous α- **lactose** monohydrate monocrystals exhibited greater mech. strength when compared with the anhydrous α- **lactose** crystals. The acoustic emission data show that the fragmentation process of the monohydrate crystals is acoustically more active and energetic. Amplitude distribution anal. of the acoustic signals further confirmed that the nature of fragmentation during the deformation of the two types of **lactose** was different. This is attributed to fundamental differences in the internal **crystal structure** of the two **lactose** types. Mech. strength and acoustic emission analyses provide an insight into the fundamental deformation characteristics of these 2 types of **lactose**.

L20 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:2418 CAPLUS
DOCUMENT NUMBER: 114:2418
TITLE: 2.2 Å Resolution structure analysis of two refined N-acetylneuraminyl-**lactose**-wheat germ agglutinin isolectin complexes
AUTHOR(S): Wright, Christine S.
CORPORATE SOURCE: Dep. Biochem. Mol. Biophys., MCV, Richmond, VA,

23298-0001, USA
SOURCE: Journal of Molecular Biology (1990), 215(4), 635-51
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The **crystal structures** of complexes of isolectins 1 and 2 of wheat germ agglutinin (WGA1 and WGA2) with N-acetylneuraminyl-**lactose** (NeuNAc-α(2-3)-Gal-β(1-4)-Glc) were refined on the basis of data in the 8-2.2 Å resolution range to final crystallog. R-factors of 17.2% and 15.3% (Fo > 1σ), resp. Specific binding interactions and water association, as well as changes in conformation and mobility of the structure upon ligand binding, were compared in the 2 complexes. The temperature factors (B = 16.3 Å2 and 18.4 Å2) were much lower compared with those of their resp. native structures (19-22 Å2). Residues involved in sugar binding, dimerization and in **lattice** contacts exhibit the largest decreases in B-value, suggesting that sugar binding reduces the overall mobility of the protein mols. in the crystal **lattice**. The binding mode of this sialyl-trisaccharide, an important cell receptor analog, was compared in the 2 isolectins. Only one of the 2 unique binding sites (4 per dimer), located in the subunit/subunit interface, is occupied in the crystals. This site, termed the primary binding site, contains one of the 5 amino acid substitutions that differentiate WGA1 and WGA2. Superposition of the refined models in each of the independent crystallog. environments indicates a close match only of the terminal non-reducing NeuNAc residue (root-mean-square Δr of 0.5-0.6 Å). The Gal-Glc portion was found to superimpose poorly, lack electron d., and possess high atomic thermal factors. In both complexes NeuNAc is stabilized through contact with 6 amino acid side-chains (Ser114 and Glu115 of subunit 1 and Ser62, Tyr64, Try(His)66, and Tyr73 of subunit 2), involving all NeuNAc ring substituents. Refinement has allowed accurate assessment of the contact distances for 4 hydrogen bonds, a strong buried non-polar contact with the acetamido CH3 group and a large number of van der Waals' interactions with the 3 aromatic side-chains. The higher affinity of N-acetylneuraminyl-**lactose** observed by NMR studies for WGA1 can be explained by the more favorable binding interactions that occur when residue 66 is a Tyr. The tyrosyl side-chain provides a larger surface for van der Waals' stacking against the NeuNAc pyranose ring than His66 and a hydrogen bond contact with Gal (C2-OH), not possible in WGA2. Saccharide-induced conformational changes in the side-chains involved in sugar binding were small but comparable in all crystallog. different complexes, and they correlate with the degree of immobilization reflected by the temperature factors.

L20 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:215684 CAPLUS
DOCUMENT NUMBER: 106:215684
TITLE: Analysis of solid structure of cellulose by CP/MAS carbon-13 NMR
AUTHOR(S): Horii, Fumitaka; Hirai, Atsuko; Kitamaru, Ryuzo
CORPORATE SOURCE: Chem. Res. Inst., Kyoto Univ., Kyoto, Japan
SOURCE: Kyoto Daigaku Nippon Kagaku Sen'i Kenkyusho Koenshu (1985), 42, 41-52
CODEN: KNKKAB; ISSN: 0368-6280
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB The mol. conformation of cellulose [9004-34-6] was studied by determining torsion angle from chemical shifts from solid-state high-resolution 13C NMR. The chemical shift was affected not only by the torsion angle but also by packing and H bond. The packing and H bond effects were discussed for cellulose-related mono- and disaccharides in terms of chemical shift and torsion angle. The 13C NMR spectra of various cellulose samples in dry state showed crystalline and noncryst. components which were distinguished by the large difference in their spin-**lattice** relaxation times. Based on these results, the mol. conformation and **crystal structure** of cellulose were discussed in terms of chemical shifts of each component. Also, the 13C NMR spectra of wet samples were analyzed similarly.

L20 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:32090 CAPLUS
DOCUMENT NUMBER: 102:32090
TITLE: Physicochemical properties of crystalline **lactose**. II. Effect of crystallinity on mechanical and structural properties
AUTHOR(S): Morita, Masami; Nakai, Yoshinobu; Fukuoka, Eihei; Nakajima, Shinichiro
CORPORATE SOURCE: Fac. Pharm. Sci., Chiba Univ., Chiba, 260, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1984), 32(10),

4076-83
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The crystal **lattice** was disordered when crystalline **lactose** α-monohydrate [64044-51-5] was dehydrated to the α-anhydrate [63-42-3] by heating in air. The disorder parameter of the α-anhydrate obtaining by desiccating α-monohydrate in MeOH was smaller than that of the product obtained by heating in air. This disorder was also induced by grinding the α-monohydrate, and the free energy level of the water of crystallization in the ground sample was higher than that in the intact sample. No structural change of amorphous **lactose** was observed at 30° in a P2O5 desiccator for 30 days. However, during storage at 30°and 60% relative humidity for 24 h, crystals of the α-monohydrate in the solid state grew and the degree of crystallinity reached approx. 75%. Further crystal growth was slight. Crystals of β-anhydrate also formed. The disorder parameter of this transformed **lactose** was larger than that of the intact sample. The degree of stress relaxation of **lactose** was small, but that of amorphous **lactose** was nearly equal to that of crystalline cellulose. The tablet hardness of amorphous **lactose** was approx. 10-fold that of crystalline **lactose**.

L20 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:28219 CAPLUS
DOCUMENT NUMBER: 100:28219
TITLE: Interpretation of the morphology of α-**lactose** hydrate
AUTHOR(S): Visser, R. A.; Bennema, P.
CORPORATE SOURCE: Res. Lab., CCF, Leeuwarden, Neth.
SOURCE: Netherlands Milk and Dairy Journal (1983), 37(3), 109-37
CODEN: NMDJAX; ISSN: 0028-209X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The morphol. of the α- **lactose** hydrate crystal was derived. The methods, which are based on the known **crystal structure**, gave exactly the same morphol. order of the faces, whereas the method, in which only the **lattice** consts. are used, gave a somewhat different result. Since, however, both results strongly deviate from the real morphol., a new method was developed, which takes into consideration the blocking of part of the growth sites by β-**lactose**. The morphol. order obtained with this method is in reasonable accordance with the observed morphol.

L20 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:419299 CAPLUS
DOCUMENT NUMBER: 97:19299
TITLE: Escherichia coli lac repressor is elongated with its operator DNA-binding domains located at both ends
AUTHOR(S): McKay, David B.; Pickover, Clifford A.; Steitz, Thomas A.
CORPORATE SOURCE: Dep. Mol. Biophys. Biochem., Yale Univ., New Haven, CT, 06511, USA
SOURCE: Journal of Molecular Biology (1982), 156(1), 175-83
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English
AB From small-angle x-ray scattering expts. on solns. of E. coli lac repressor and repressor tryptic core, it was concluded that the domains of repressor that bind to operator DNA lie at the ends of an elongated mol. The addition of the inducer, isopropyl-β-D-thiogalactoside (I), to either repressor or core did not produce a measurable structural change, since the radius of gyration of repressor was 40.3 Å without and 42.2 Å with I; the core radius of gyration was 35.4 Å without ligand and 36.3 Å with I. From data from **single crystals** of repressor and core, the measured radii of gyration were shown to be consistent with a core (or repressor) mol. of dimensional anisotropy 1:(1.5-2.0):(3.0-4.0). The 5 Å difference in radius of gyration between native and core repressor was interpreted to mean that the amino terminal 59 residues (headpieces) lie at the ends of an elongated repressor mol. This structure implies that the repressor may have DNA binding sites, consisting of 2 adjacent headpieces, on each end of the mol., and this binds to the DNA with its long axis perpendicular to the DNA.

L20 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:2838 CAPLUS

DOCUMENT NUMBER: 94:2838
TITLE: Crystallographic elucidation of the saccharide binding mode in wheat germ agglutinin and its biological significance
AUTHOR(S): Wright, Christine Schubert
CORPORATE SOURCE: Dep. Biochem. Sci., Princeton Univ., Princeton, NJ, 08540, USA
SOURCE: Journal of Molecular Biology (1980), 141(3), 267-91
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fourier anal. of wheat germ agglutinin (WGA)-sugar complexes indicated that all 4 domains (A, B, C, D) of each WGA protomer (I and II) contributed to sugar binding at 4 locations in the protomer/protomer contact region: BI/CII, BII/CI, AI/DII, AII/DI. The 2 equivalent binding sites involving the B and C domains which bind N-acetylneuraminic acid, termed the primary binding location, were readily accessible in the crystal to all 3 saccharides tested: di-N-acetylglucosamine, 6-iodo-1,4-dimethyl-N-acetylglucosamine, and N-acetylneuraminic acid-**lactose**. The other 2 sites involving A and D domains were termed the secondary binding locations since they were only poorly occupied by di-N-acetylglucosamine in glutaraldehyde-crosslinked crystals and not at all by the sialic acid sugars. The binding modes at the 2 binding locations are presented and discussed. Thus, differing accessibility and specificity determinants for the 2 unique binding sites in WGA, as well as protein self-association as seen in the crystal **lattice**, could explain the cooperative binding behavior of WGA binding to various cells, and the rapid release of cell bound WGA when N-acetylglucosamine is introduced.

L20 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:517649 CAPLUS
DOCUMENT NUMBER: 89:117649
TITLE: Stability of **lattice** dislocations. Thermal deactivation of organic solids
AUTHOR(S): Huettenrauch, R.; Keiner, Ingeburg
CORPORATE SOURCE: Wiss. Lab., VEB Jenapharm, Jena, Hung.
SOURCE: Pharmazie (1978), 33(6), 376-7
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German

AB The stability of structural defects in **lactose** [63-42-3] and powdered cellulose [9004-34-6] was studied at room temperature and after tempering. The **lattice** dislocations (mech. induced crystallinity changes, 16.5% in **lactose** and 26% in powdered cellulose) were not decreased by storage under ambient conditions for 3 mo. However, **lactose** ground in a hammer mill and then stored at room temperature, 60° and 80° showed no crystallinity changes during the first 40 days. Thereafter, the **lattice** dislocations increased, crystallinity decreased to 76% and remained at this level for ≤70 days. The response of activated powdered cellulose to tempering was similar to that of metals and plastics. Recrystn. started within the first h, was 4% after 20 h, and occurred more rapidly at higher temps. Complete recrystn. was not always achieved. Comparison of the behavior of **lactose** and cellulose shows that the effect of tempering depends on the type of **crystal structure**, the composition, and possibly on the type of **lattice** defects.

L20 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:582369 CAPLUS
DOCUMENT NUMBER: 85:182369
TITLE: Molecular galenics. Part 14. Mechanisms of tableting
AUTHOR(S): Huettenrauch, R.; Keiner, Ingeburg
CORPORATE SOURCE: Wiss. Lab., VEB Jenapharm, Jena, Ger. Dem. Rep.
SOURCE: Pharmazie (1976), 31(9), 651-2
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German

AB α- **Lactose**-H2O [14641-93-1] yielded harder tablets on compression than did β- **lactose** [63-42-3]. Both anomers formed monoclinic crystals, but the crystals had different cell dimensions and **lattice** energies for the 2 anomers. β- **Lactose** had the greater d. and therefore underwent surface activation less readily. These results suggested that surface activation during compression may result in localized sintering and thus account for the adherence of particles in tablets.

L20 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:408146 CAPLUS
DOCUMENT NUMBER: 57:8146
ORIGINAL REFERENCE NO.: 57:1653f
TITLE: Structure of α- **lactose** monohydrate (milk sugar)
AUTHOR(S): Seifert, H.; Labrot, G.
CORPORATE SOURCE: Univ. Muenster, Germany
SOURCE: Naturwissenschaften (1961), 48, 691
CODEN: NATWAY; ISSN: 0028-1042
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB **Lactose** is monoclinicsphenoidic, with Z = 2.03 for exptl. d. 1.497. The space group is C22-P21 with a 7.86 ± 0.01, b 21.894 ± 0.02, c 4.897 ± 0.01 A., β 105°58.5' ± 1'. **Lattice** data d [100] = d[101] = 8.04 A. are given.

L20 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1958:41960 CAPLUS
DOCUMENT NUMBER: 52:41960
ORIGINAL REFERENCE NO.: 52:7557d-e
TITLE: Methods of identification and of finding the quantitative ratios of α- and β- **lactose** [in mixtures thereof]
AUTHOR(S): Kovalenko, M. S.
SOURCE: Trudy Leningrad. Tekhnol. Inst. Kholodil. Prom. (1956), 14, 210-14
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The changes in electroconductivities of aqueous solns. effected by the addition of H3BO3 and the **lattice** constant d found from a Debye-Scherrer diagram are used as methods of identification and determination The latter method is especially suitable, as d = 7.32 A. for α- **lactose** and 8.57 A. for β- **lactose**, and mixts. will show a linear relation for the d-value observed.